



Combined  
Error and  
Uncertainty

Tim Barth

Non-  
Intrusive  
Methods

An Error  
Bound on  
Statistics

Numerical  
Results

# Combined Uncertainty and A-Posteriori Error Bound Estimates for CFD Calculations: Theory and Implementation

Tim Barth

NASA Ames Research Center  
Moffett Field, California 94035 USA  
([Timothy.J.Barth@nasa.gov](mailto:Timothy.J.Barth@nasa.gov))

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# Introduction

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Simulation codes often utilize finite-dimensional approximation resulting in **numerical error**. Some examples include

- numerical methods utilizing grids and finite-dimensional basis functions,
- particle methods using a finite number of particles.

These same simulation codes also often contain **sources of uncertainty**, for example

- uncertain parameters and fields associated with the imposition of initial and boundary data,
- uncertain physical model parameters such as chemical reaction rates, mixture model parameters, material property parameters, etc.

*Remark:* Another form of error amenable to the present analysis (but not considered here) is **modeling error**, e.g. approximate models of turbulence, chemical catalysis, and radiation.



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**Non-intrusive uncertainty quantification methods** quantify the uncertainty of output quantities of interest (QoI) by performing simulation realizations for specific values of uncertain parameters.

Question: How does realization error effect moment statistics calculated using these non-intrusive methods?

To address this question, we have constructed computable *a posteriori* error bounds for output QoI moment statistics such as expectation  $E[\cdot]$  and variance  $V[\cdot]$ .

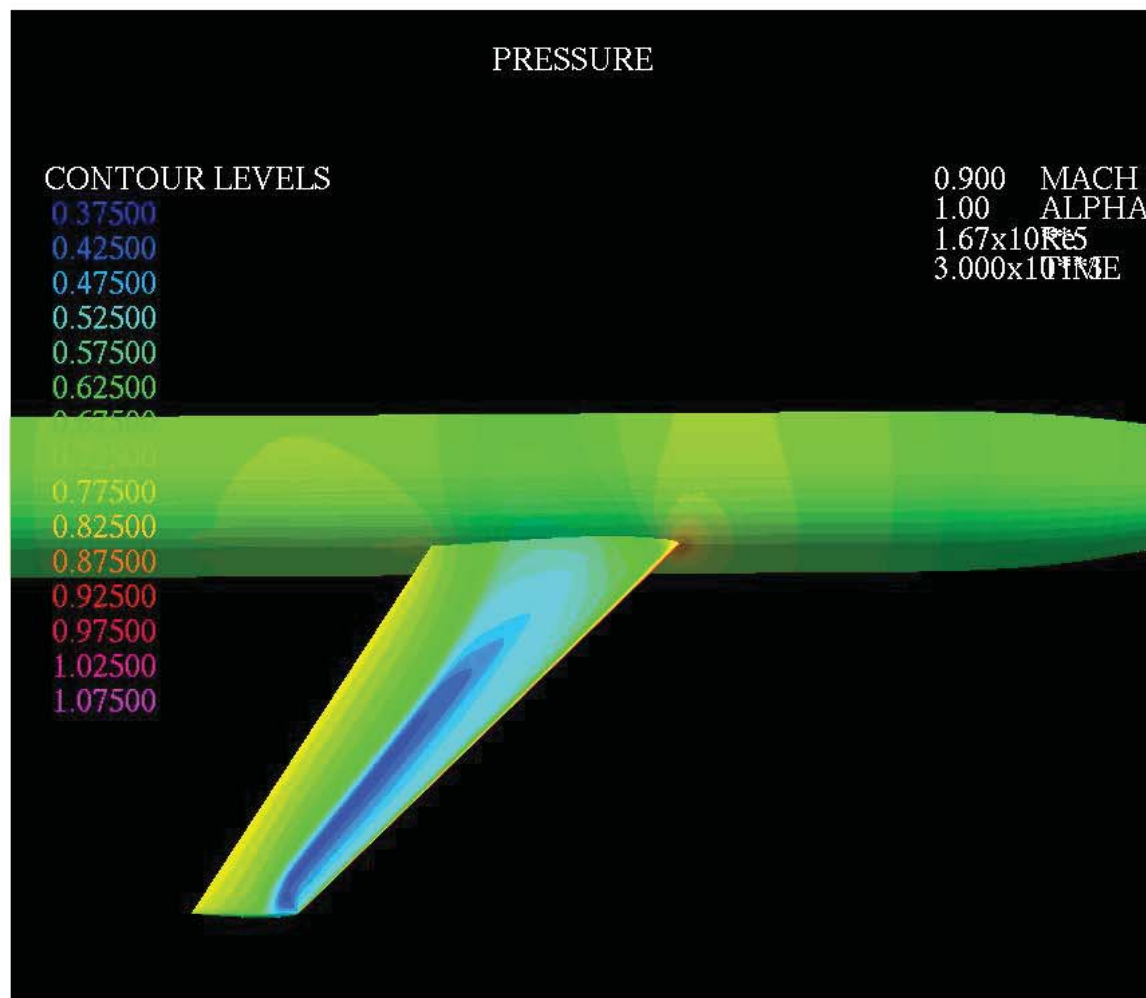
$$E[f] = \int_{\Xi} f(\xi) p(\xi) d\xi \quad , \quad V[f] = \int_{\Xi} (f(\xi) - E[f])^2 p(\xi) d\xi \quad .$$



# Preview Example: Uncertainty Calculation with Error Bounds

Software!

- Wing-body CFD calculations using the Reynolds-averaged Navier-Stokes equations,
- 2-equation turbulence model,
- Flight Mach number uncertainty,  $M_\infty = \text{Gaussian}_{3\sigma}(m = .9, \sigma = .0225)$ ,
- Hybrid Glenshaw-Curtis calculation of moment statistics.







# Uncertainty Quantification for Output Quantities of Interests

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Let  $\alpha \in \mathbf{R}^N$  denote a vector of  $N$  uncertain parameter associated with sources of uncertainty,  $u_h(x, t; \alpha)$  a numerical realization in  $(x, t) \in \mathbf{R}^{d+1}$  with uncertain parameters  $\alpha$ , and  $u(x, t; \alpha)$  the exact infinite-dimensional counterpart.

Quantities of Interest (QoI). Let  $J(u_h; \alpha) \equiv J(u_h(x, t; \alpha); \alpha)$ ; denote an output quantity of interest

- Functionals such as space-time integrated forces and moments.
- Graphs of derived quantities such as pressure or temperature along a space-time curve.
- Derived quantities from general space-time volume subsets.

Non-intrusive uncertainty propagation. The non-intrusive propagation methods considered herein obtain estimates of QoI statistics and/or probability densities from  $M$  realization QoI outputs

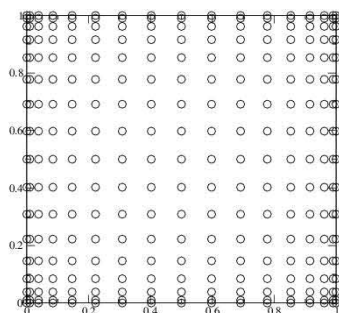
$$\{J(u_h; \alpha^{(1)}), J(u_h; \alpha^{(2)}), \dots, J(u_h; \alpha^{(M)})\}$$



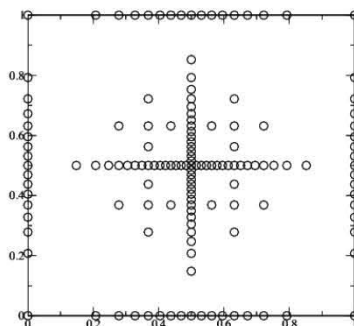
# Calculation of Moment Statistics via Quadrature

Let  $N$  denote the number of uncertainty (stochastic) dimensions

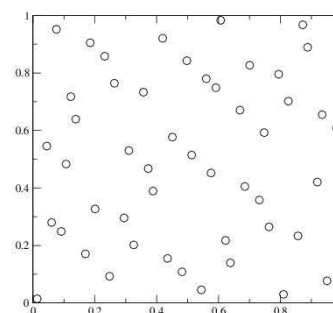
- **Dense tensorization methods**, complexity  $\mathcal{O}(M_{1D}^N)$ 
  - Stochastic collocation, precision  $2M_{1D} - 1$ , smooth integrands
  - Multilevel Clenshaw-Curtis and Gauss-Patterson quadratures,  $M_{1D} = 2^{level} \pm 1$ , precision  $2^{level} + 1$ , smooth integrands
  - Hybrid Multi-level Clenshaw-Curtis and Adaptive Polynomial (HYGAP) quadrature, Barth (2011), piecewise smooth integrands
- **Sparse tensorization methods**, complexity  $\mathcal{O}(N^{precision})$ 
  - Clenshaw-Curtis and Gauss-Patterson Sparse Grids, precision  $2^{level} + 1$ , smooth integrands
- **Multi-Level (M-L) sampling methods**
  - Multi-level random sampling for hyperbolic stochastic conservation laws (Mishra and Schwab (2009)), smooth and non-smooth integrands



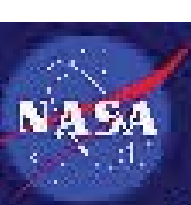
Dense Tensor



Sparse Tensor



Sampling



# Quadrature Complexity

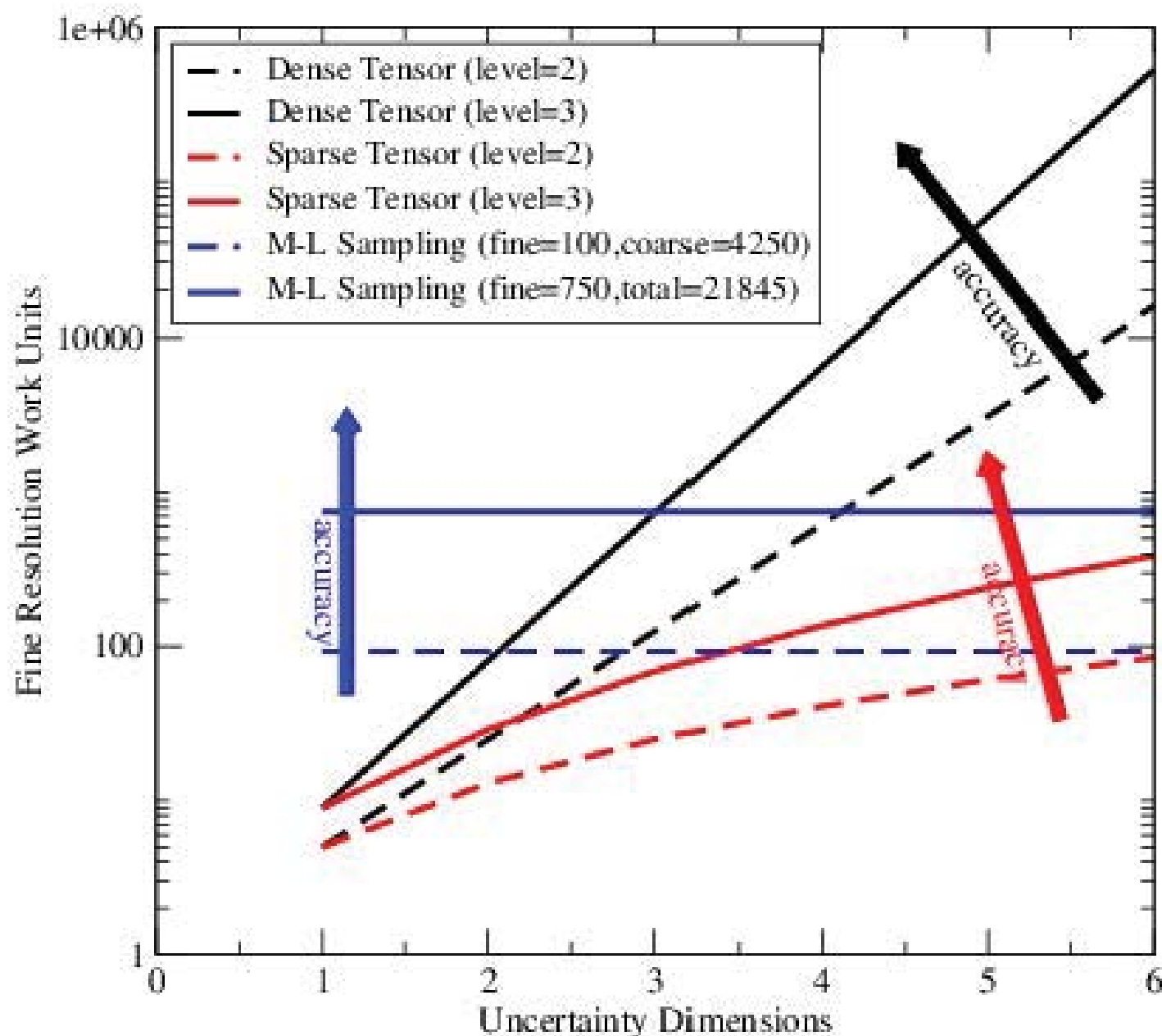
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# An Error Bound for Moment Statistics with Realization Error – Preliminaries

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Let  $I[f]$  denote the weighted **definite integral**

$$I[f] = \int_{\Xi} f(\xi) p(\xi) d\xi, \quad p(\xi) \geq 0$$

and  $Q_M I[f]$  denote an  $M$ -point weighted **numerical quadrature**

$$Q_M I[f] = \sum_{j=1}^M w_j f(\xi_j)$$

with weights  $w_j$  with evaluation points  $\xi_j$ . Finally, define numerical **quadrature error** denoted by  $R_M I[f]$ , i.e.

$$R_M I[f] = I[f] - Q_M I[f].$$





# An Error Bound for Moment Statistics with Realization Error

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Let  $\epsilon = J(u) - J(u_h)$  denote the QoI error.

## Expectation Error

$$|E[J(u)] - Q_M E[J(u_h)]| \leq |Q_M E[|\epsilon|]| + |R_M E[|\epsilon|]| + |R_M E[J(u_h)]|$$

## Variance Error

$$\begin{aligned} |V[J(u)] - Q_M V[J(u_h)]| &\leq 2 \left( (|Q_M E[|\epsilon|^2]| + |R_M E[|\epsilon|^2]|) \right. \\ &\quad \times (|Q_M V[J(u_h)]| + |R_M V[J(u_h)]|) \Big)^{\frac{1}{2}} \\ &\quad + |Q_M E[|\epsilon|^2]| + |R_M E[|\epsilon|^2]| + |R_M V[J(u_h)]|. \end{aligned}$$

- **Red** terms can be made smaller by decreasing realization error,  $\downarrow \epsilon$ .
- $R_M E[\cdot]$  and  $R_M V[\cdot]$  can be made smaller by increasing  $M$ ,  $\uparrow M$ .



# The Adaptivity Framework

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Adaptivity Framework Objective: Answer adaptivity query questions (approximately) **without explicitly computing new realizations.**

- Estimate the effect of solving the given realizations more or less accurately by multiplying the QoI error at the  $M$  realization quadrature points by a factor  $e_j, j = 1, \dots, M$ , e.g. let  $e \in [0, 1]^M$

$$Q_M E[|\epsilon|](e) \equiv \sum_{j=1}^M w_j e_j \epsilon_j$$

- Estimate the effect of solving the numerical quadratures more or less accurately by exposing the dependence of the quadrature error on the parameter  $M$ . Let  $M'$  denote a proposed new quadrature parameter, estimate the expected decrease/increase in quadrature error, e.g.

$$R_M E[\cdot](q) \equiv f(q) R_M E[\cdot], \quad q = M' / M$$

with  $f(q)$  the predicted quadrature error decrease/increase (derived later on).



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Expectation error formula with adaptivity parameters  $(e, q)$

$$|E[J(u)] - Q_M E[J(u_h)]|(e, q) \leq |Q_M E[|\epsilon|]|(e) + |R_M E[|\epsilon|]|(e, q) + |R_M E[J(u_h)]|(q)$$

Scenarios

- **(Analysis)** Calculate the accuracy of computed statistics. Set  $q = 1, e_i = 1$ .
- **(Error Balancing)** Given realizations with error  $\epsilon$ , determine the value of  $q = M'/M$  that balances the error terms

$$|Q_M E[|\epsilon|]| = |R_M E[J(u_h)]|(q) + |R_M E[|\epsilon|]|(1, q)$$

For  $q > 1$ , new realization must be performed.

- **(Error Balancing with Specified Error Level)** Specify a given level of error,  $\delta$ , for QoI statistics, determine  $q$  and  $e$  such that

$$\delta/2 = |Q_M E[|\epsilon|]|(e) = |R_M E[J(u_h)]|(q) + |R_M E[|\epsilon|]|(e, q) .$$

If  $q > 1$ , new realizations must be performed. If  $e_i < 1$ , then realization  $i$  must be solved more accurately.



# Computable Error Bound Estimates – Remaining Tasks

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Estimate the quadrature error,  $R_M[\cdot] \equiv I[\cdot] - Q_M[\cdot]$ , arising from the calculation of statistics.

- (dense and sparse quadratures) Exploit the node-nested structure of multi-level Clenshaw-Curtis and Gauss-Patterson quadrature.
- (multi-level sampling) Use the well-known quadrature error formula for Monte-Carlo sampling,  $Q_M E[f] \propto M^{-1/2}$  (not discussed here).





# Multi-level Node-Nested Quadrature

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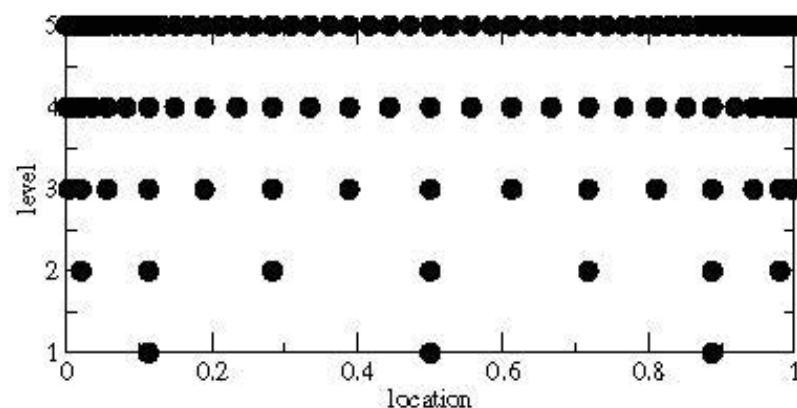
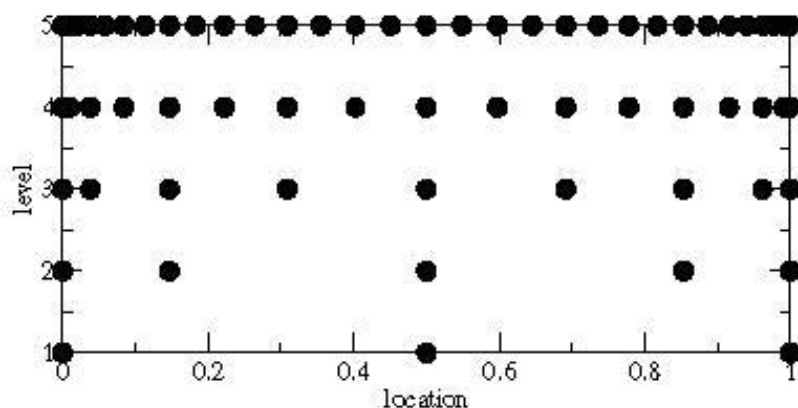
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Multi-level node-nested quadratures such as Clenshaw-Curtis and Gauss-Patterson quadrature provide a particularly advantageous framework for estimating moment statistics and estimating the underlying quadrature error.

- Used in both dense and sparse tensorization,
- $2^{level} + 1$  polynomial precision,
- Data at level  $L$  reuses all data at level  $L - 1$ ,
- Combined with piecewise polynomial approximation in the HYGAP algorithm (Barth, 2011) for piecewise smooth integrands.



*Node-nested Clenshaw-Curtis (left) and Gauss-Patterson (right) quadrature point locations.*



# Clenshaw-Curtis and Gauss-Patterson Quadrature Error Estimates

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Integral in  $\mathbf{R}^d$

$$I[f] = \int_{[0,1]^d} f(\xi) d\xi$$

Sparse quadrature formula (Smolyak) given a 1-D quadrature  $Q_i^{(1)}[\cdot]$

$$Q_L^{(d)} I[f] = \left( \sum_{j=1}^L \left( Q_j^{(1)} - Q_{j-1}^{(1)} \right) \otimes Q_{L-j+1}^{(d-1)} \right) I[f] .$$

Error estimate for  $L$ -level Clenshaw-Curtis and Gauss-Patterson sparse quadrature in  $\mathbf{R}^d$  for integrands with  $r$  regularity,  $f \in C^r$

$$|R_L^{(d)} I[f]| = \mathcal{O} \left( M_L^{-r} (\log(M_L))^{(d-1)(r+1)} \right) .$$

This error formula correctly reproduces the known 1-D error estimate for Clenshaw-Curtis and Gauss-Patterson quadrature

$$|R_L^{(1)} I^{(1)}[f]| = \mathcal{O}(2^{-rL}) .$$



# Computable Sparse and Dense Quadrature Error Estimates—Estimate A

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Error estimate for  $L$ -level sparse quadrature in  $\mathbf{R}^d$  for integrands with  $r$  regularity<sup>1</sup>.

$$|R_L^{(d)} I[f]| = \mathcal{O} \left( M_L^{-r} (\log(M_L))^{(d-1)(r+1)} \right).$$

**Estimate A (3-Level).** Evaluate the quadrature error formula for 3 levels

- ①  $I[f] - Q_L^{(d)} I[f] = C M_L^{-r} (\log(M_L))^{(d-1)(r+1)} + h.o.t.$
- ②  $I[f] - Q_{L-1}^{(d)} I[f] = C M_{L-1}^{-r} (\log(M_{L-1}))^{(d-1)(r+1)} + h.o.t.$
- ③  $I[f] - Q_{L-2}^{(d)} I[f] = C M_{L-2}^{-r} (\log(M_{L-2}))^{(d-1)(r+1)} + h.o.t.$

Ignoring higher-order terms, this is a system of 3 equations in the 3 unknowns  $\{I[f], C, r\}$  subject to regularity limits  $r \in [r_{min}, r_{max}]$ .

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<sup>1</sup> Shorthand notation:  $R_L I[f] \equiv R_{M_L} I[f]$





# Computable Sparse and Dense Quadrature Error Estimates—Estimate B

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**Estimate R** (2-Level,  $r$  parameter). Evaluate the quadrature error formula for 2 levels assuming  $r$  is *given*

$$\textcircled{1} \quad I[f] - Q_L^{(d)} I[f] = C M_L^{-r} (\log(M_L))^{(d-1)(r+1)} + h.o.t.$$

$$\textcircled{2} \quad I[f] - Q_{L-1}^{(d)} I[f] = C M_{L-1}^{-r} (\log(M_{L-1}))^{(d-1)(r+1)} + h.o.t.$$

Explicitly solve for the quadrature error,  $R_L^{(d)} I[f]$

$$I[f] - Q_L^{(d)} I[f] \equiv R_L^{(d)} I[f] = \frac{(Q_L^{(d)} I[f] - \beta_L(r) Q_{L-1}^{(d)} I[f])}{1 - \beta_L(r)} - Q_L^{(d)} I[f]$$

with

$$\beta_L(r) \equiv \frac{M_L^{-r} \log^{(d-1)(r+1)}(M_L)}{M_{L-1}^{-r} \log^{(d-1)(r+1)}(M_{L-1})}.$$

Liu, Gao, and Hesthaven (2011) claim that for smooth functions, “*the error estimator has limited sensitivity to  $r$  and we have found that taking it to values of 2-4 generally yields excellent results*” although their results do not provide convincing evidence of this.





# Computable Sparse and Dense Quadrature Error Estimates—Estimate C

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**Estimate E (3-Level).** Estimate the quadrature error using a 3-Level extrapolation formula

$$\log(I[f] - Q_{M_L} I[f]) = 2 \log(Q_{M_L} I[f] - Q_{M_{L-1}} I[f]) - \log(Q_{M_{L-1}} I[f] - Q_{M_{L-2}} I[f])$$

The regularity and constant,  $\{r, C\}$  can then estimated from

- ①  $I[f] - Q_L^{(d)} I[f] = C M_L^{-r} (\log(M_L))^{(d-1)(r+1)}$
- ②  $I[f] - Q_{L-1}^{(d)} I[f] = C M_{L-1}^{-r} (\log(M_{L-1}))^{(d-1)(r+1)}$

This gives an explicit quadrature error formula for the **Adaptivity Framework**

$$R_M E[\cdot](q) \equiv f(q) R_M E[\cdot], \quad q = M_{L'}/M_L$$

with

$$f(q) = \frac{M_{L'}^{-r} (\log(M_{L'}))^{(d-1)(r+1)}}{M_L^{-r} (\log(M_L))^{(d-1)(r+1)}}$$



# Sparse Quadrature Error Estimate: Example Calculation

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## 5-Dimensional Integral

$$\int_{[0,1]^5} \prod_{i=1}^d \sin(\pi \xi_i) d\xi = 2^5$$

## Clenshaw-Curtis Sparse Tensor Quadrature Estimates

level	quadrature	true error	Est A	(r=5.5) Est R	(r=4.0) Est R	Est E
3	90.32273573	58.3	-	-	-	-
4	37.60810455	5.60	-	22.30	37.22	-
5	29.15399282	-2.84	3.2	9.96E-1	2.04	1.35
6	31.77676498	-2.23E-1	-1.23	-1.83E-1	-4.17E-1	8.13E-1
7	32.04908081	4.91E-2	-1.03E-1	-1.40E-2	-3.42E-2	2.82E-2
8	32.00861824	8.61E-3	2.10E-1	1.72E-3	4.38E-3	6.01E-3
9	32.00056238	5.62E-4	4.92E-3	3.01E-4	7.88E-4	1.60E-3
10	32.00001861	1.86E-5	3.01E-4	1.84E-5	4.94E-5	3.65E-5
11	32.00000033	3.31E-7	1.02E-5	5.78E-7	1.57E-6	6.15E-7



# Error Bound Estimates – Remaining Tasks

Software!

Estimate  $|\epsilon_h^{(i)}| \equiv |J(u; \alpha^{(i)}) - J(u_h; \alpha^{(i)})|$  for each realization  $i$ . Some viable techniques include

- Richardson (2-level) and Aitken (3-level) extrapolation using space-time grid hierarchies,
- Error evolution, see for example the work of Jeff Banks at LLNL,
- Patch postprocessing techniques: Zienkiewicz-Zhu, Bramble-Schatz, Cockburn *et. al.*,
- *A posteriori* error estimation of functionals using dual / adjoint problems



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## Further Numerical Results





# A Model PDE Problem with Uncertainty and Error Specification

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**Deterministic Burgers' Problem:** Viscosity-free Burgers' equation

$$\frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} (u^2(x, t)/2) = 0, \quad (x, t) \in [0, 1] \times [0, T]$$

with sinusoidal initial data

$$u(x, 0) = \sin(2\pi x) .$$

**Phase Uncertain Burgers' Problem:** Introduce a random variable,  $\omega$

$$\frac{\partial}{\partial t} u(x, t, \omega) + \frac{\partial}{\partial x} (u^2(x, t, \omega)/2) = 0, \quad (x, t, \omega) \in [0, 1] \times [0, T] \times \mathcal{P}$$

with phase uncertain initial data

$$u(x, 0, \omega) = \sin(2\pi(x + g(\omega))) .$$

- $g(\omega) = \sin(2\pi\omega)/10$  in present calculations,
- Probability density,  $p(\omega)$ : Gaussian <sub>$\sigma=3$</sub> ( $\mu = 0, \sigma = 0.07$ ),
- WENO finite-volume (cubic polynomials) used in numerical calculations,
- Clenshaw-Curtis Adaptive Polynomial quadrature used for statistics,  $M = 9$ ,
- An exact solution is readily obtained,  $u(x, t, \omega) = u(x + g(\omega), t)$  for use in specifying the exact realization error.



# Burgers' Equation with Phase Uncertain Initial Data

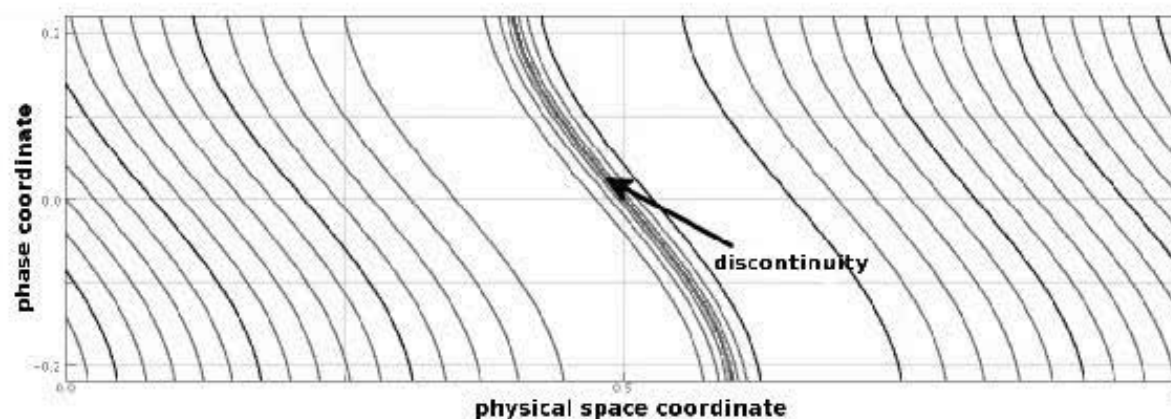
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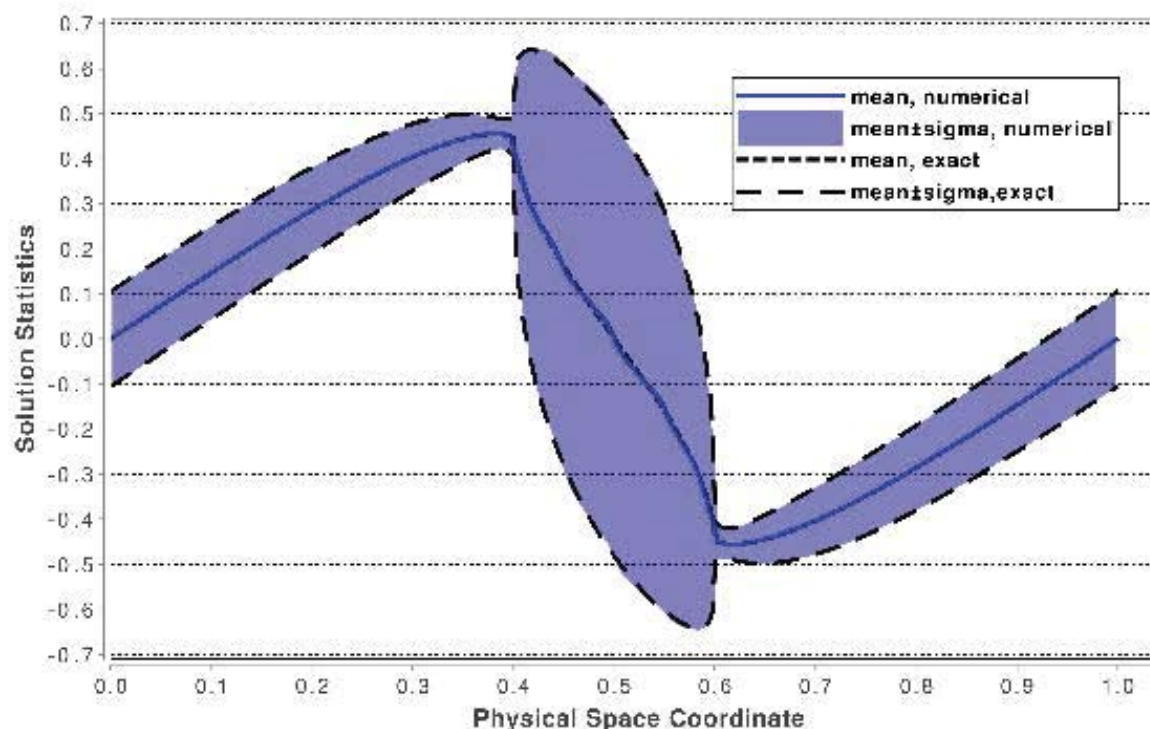
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**Solution contours at time  $t = .35$**



**Moment statistics at time  $t = .35$**



# Burgers' Equation with Phase Uncertain Initial Data

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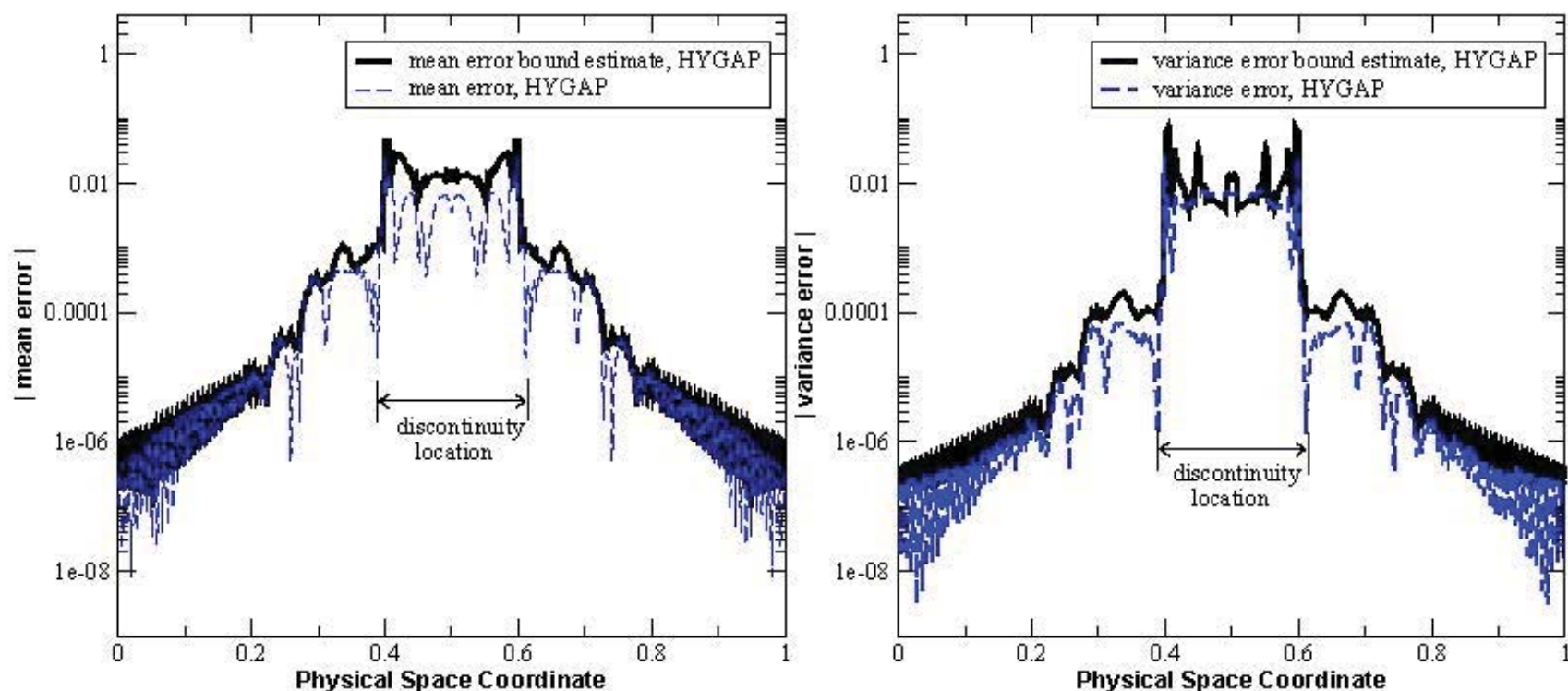


Figure : Exact and estimated error bounds for the variance statistic calculated using a Clenshaw-Curtis Adaptive Polynomial (HYGAP) approximation ( $M = 9$ ) at Clenshaw-Curtis quadrature points for the Burgers' equation problem with phase uncertain initial data at time  $t = .35$ .





# Uncertainty Quantification of Functionals: Error Representation via Dual Problems

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Semilinear form  $\mathcal{B}(\cdot, \cdot)$  and nonlinear  $J(\cdot)$ .

Primal numerical problem: Find  $\mathbf{u}_h \in \mathcal{V}_h$  such that

$$\mathcal{B}(\mathbf{u}_h, \mathbf{w}_h) = F(\mathbf{w}_h) \quad \forall \mathbf{w}_h \in \mathcal{V}_h.$$

Linearized auxiliary dual problem: Find  $\Phi \in \mathcal{V}$  such that

$$\overline{\mathcal{B}}(\mathbf{w}, \Phi) = \overline{J}(\mathbf{w}) \quad \forall \mathbf{w} \in \mathcal{V}.$$

$$\begin{aligned} J(\mathbf{u}) - J(\mathbf{u}_h) &= \overline{J}(\mathbf{u} - \mathbf{u}_h) && \text{(mean value } J) \\ &= \overline{\mathcal{B}}(\mathbf{u} - \mathbf{u}_h, \Phi) && \text{(dual problem)} \\ &= \overline{\mathcal{B}}(\mathbf{u} - \mathbf{u}_h, \Phi - \pi_h \Phi) && \text{(Galerkin orthogonality)} \\ &= \mathcal{B}(\mathbf{u}, \Phi - \pi_h \Phi) - \mathcal{B}(\mathbf{u}_h, \Phi - \pi_h \Phi) && \text{(mean value } \mathcal{B}) \\ &= F(\Phi - \pi_h \Phi) - \mathcal{B}(\mathbf{u}_h, \Phi - \pi_h \Phi), && \text{(primal problem)} \end{aligned}$$

Final error representation formula:

$$J(\mathbf{u}) - J(\mathbf{u}_h) = F(\Phi - \pi_h \Phi) - \mathcal{B}(\mathbf{u}_h, \Phi - \pi_h \Phi)$$





# Error Estimation of Functionals: Multi-Element Airfoil

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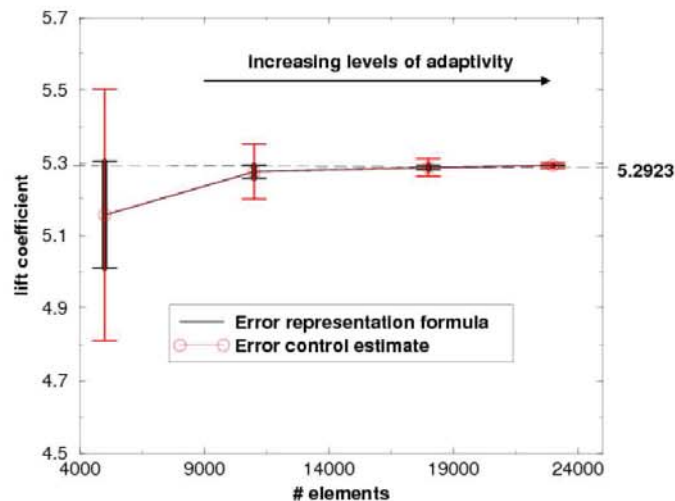
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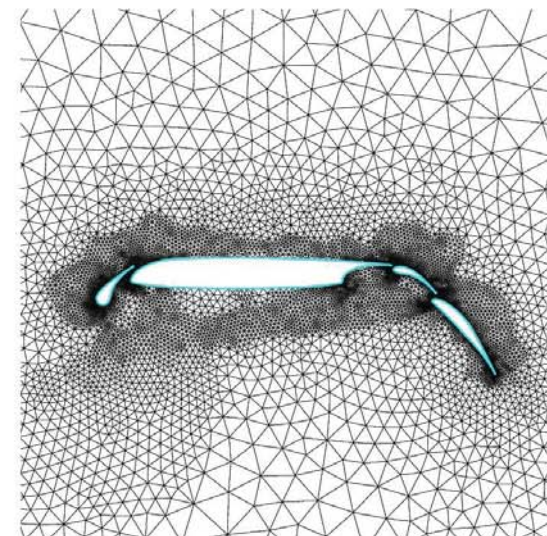
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**Example:** Euler equation flow past multi-element airfoil geometry.  
 $M = .1$ ,  $5^\circ$  AOA.

lift coefficient (error representation)	lift coefficient (error control)	refinement level	# elements	equivalent uniform refinement # elements
$5.156 \pm .147$	$5.156 \pm .346$	0	5000	5000
$5.275 \pm .018$	$5.275 \pm .076$	1	11000	20000
$5.287 \pm .006$	$5.287 \pm .024$	2	18000	80000
$5.291 \pm .002$	$5.291 \pm .007$	3	27000	320000



Error reduction during mesh adaptivity



Adapted mesh (18000 elements)



# Uncertainty of Functionals: Multi-Element Airfoil

Combined  
Error and  
Uncertainty

Tim Barth

Non-  
Intrusive  
Methods

An Error  
Bound on  
Statistics

Numerical  
Results

The inflow angle of attack (AOA) is then assumed uncertain with truncated Gaussian probability density,  $\text{AOA} = \text{Gaussian}_{4\sigma}(m = 5^\circ, \sigma = 1^\circ)$ .

Let

$$\Delta_M E[J(\mathbf{u})] \equiv E[J(\mathbf{u})] - Q_M E[J(\mathbf{u}_h)] \quad , \quad \Delta_M V[J(\mathbf{u})] \equiv V[J(\mathbf{u})] - Q_M V[J(\mathbf{u}_h)]$$

denote the errors in approximated expectation and variance, respectively using Clenshaw-Curtis quadrature ( $M=9$ ).

level	# elements	$E[J(u_h)]$	$V[J(u_h)]$	$\Delta_M E[J(u_h)]$	$\Delta_M V[J(u_h)]$
0	5000	5.145	.01157	.147	.05619
1	11000	5.274	.01188	.018	.00462
2	18000	5.286	.01191	.006	.00240
3	32000	5.292	.01192	.005	.00148

Table : Approximated statistics and error bounds for the aerodynamic lift coefficient functional. Tabulated are the computed estimates of expectation and variance together with error bounds.

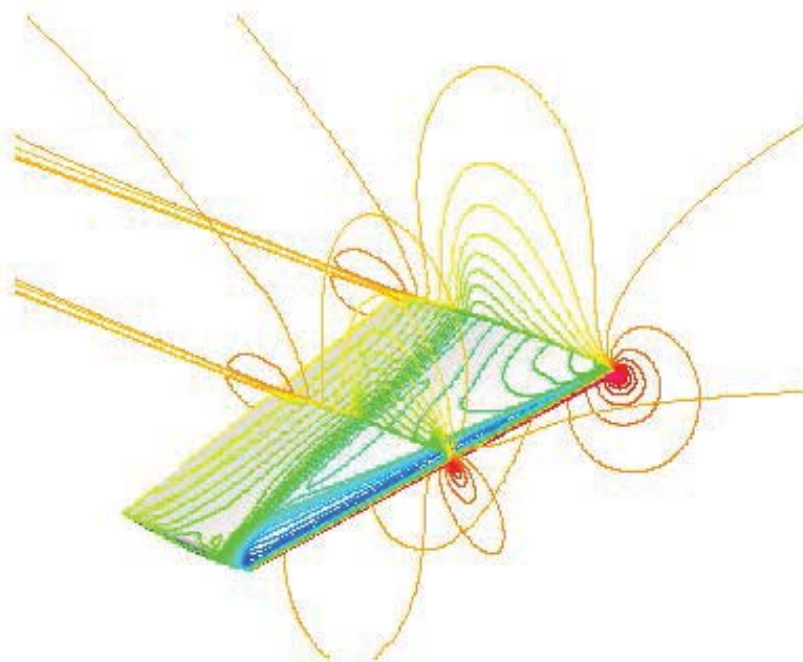




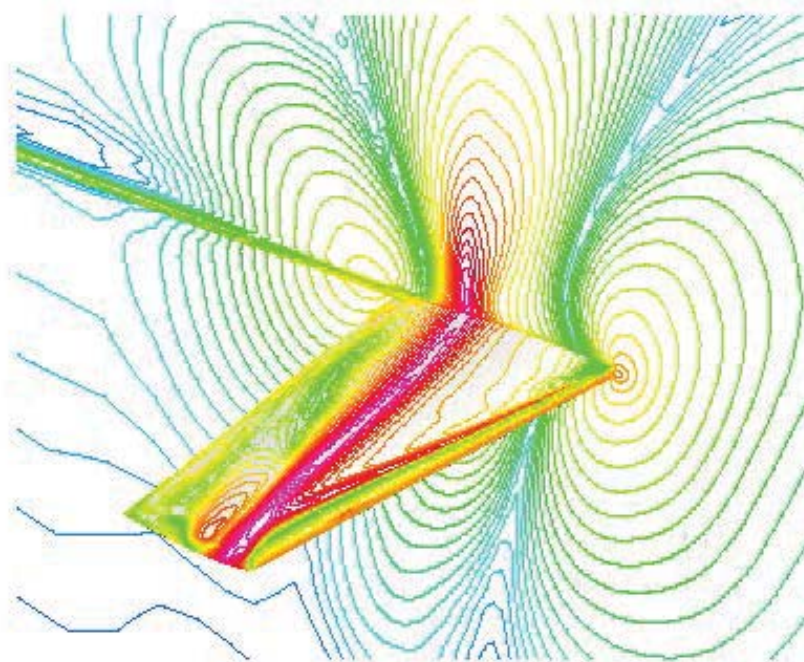
# Example Calculation: ONERA M6 Wing

Software!

- Compressible Navier-Stokes CFD calculation,
- 2-equation turbulence model,
- Inflow Mach number uncertainty,  $M_\infty = \text{Gaussian}_{3\sigma}(m = .84, \sigma = .02)$
- Angle of Attack uncertainty,  $AOA = \text{Gaussian}_{3\sigma}(m = 3.06, \sigma = .075)$
- Hybrid Clenshaw-Curtis Adaptive Polynomial quadrature ( $M=9 \times 9$ ).



expectation(density)



$\log_{10} \text{variance}(\text{density})$



# Ongoing Work – Beyond Moment Statistics

Combined  
Error and  
Uncertainty

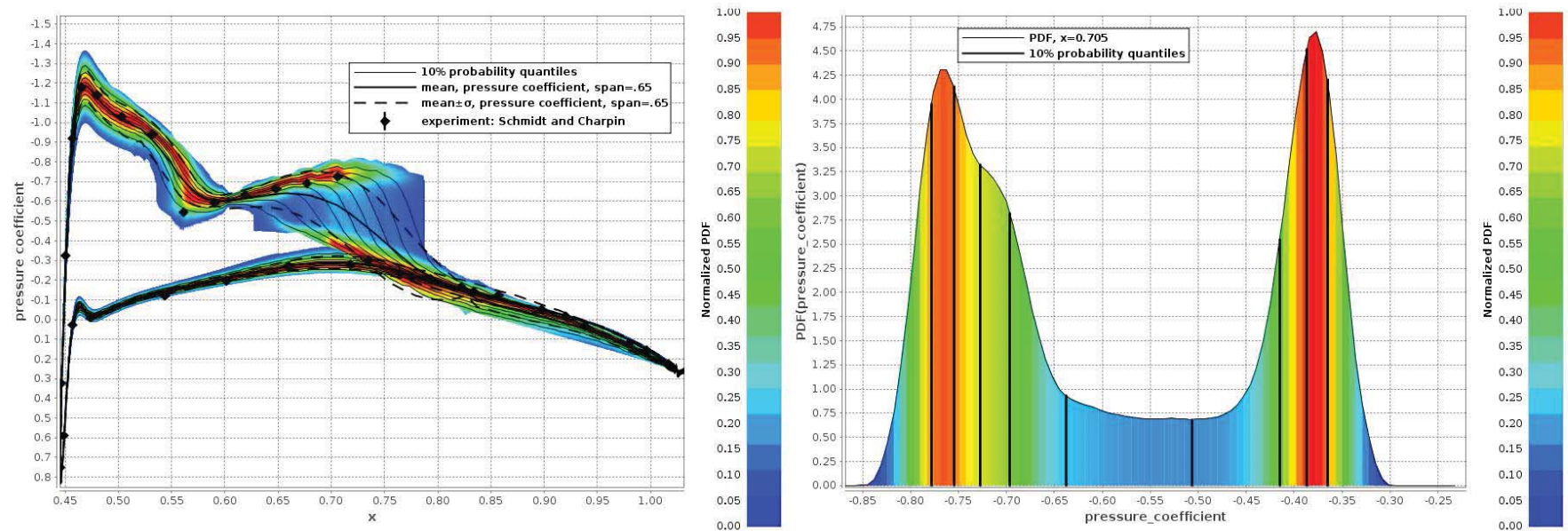
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- Moment statistics have a limited value whenever the output PDF departs strongly from a normal distribution.



PDF and Quantiles at span=.65 (left)

Bi-modal PDF at x=.705 (right)

Ongoing work:

- Calculation of non-moment statistics, e.g. PDFs, quantiles, etc.
- Error bounds for non-moment statistics.





# Concluding Remarks

Combined  
Error and  
Uncertainty

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Quantifying the effect of realization error in the calculation of output moment statistics is a novel new capability not found elsewhere.

The Adaptivity Framework and software API opens exciting new possibilities in adaptive CFD calculations.

Moving beyond moment statistics towards the estimation of error bounds for more general statistical measures and PDFs is a vitally important capability that must be provided in order that UQ is genuinely useful to engineers.